Higher Order Structures for Graph Explanations

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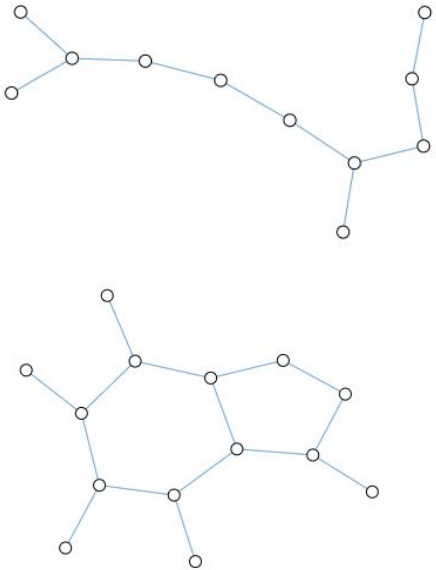
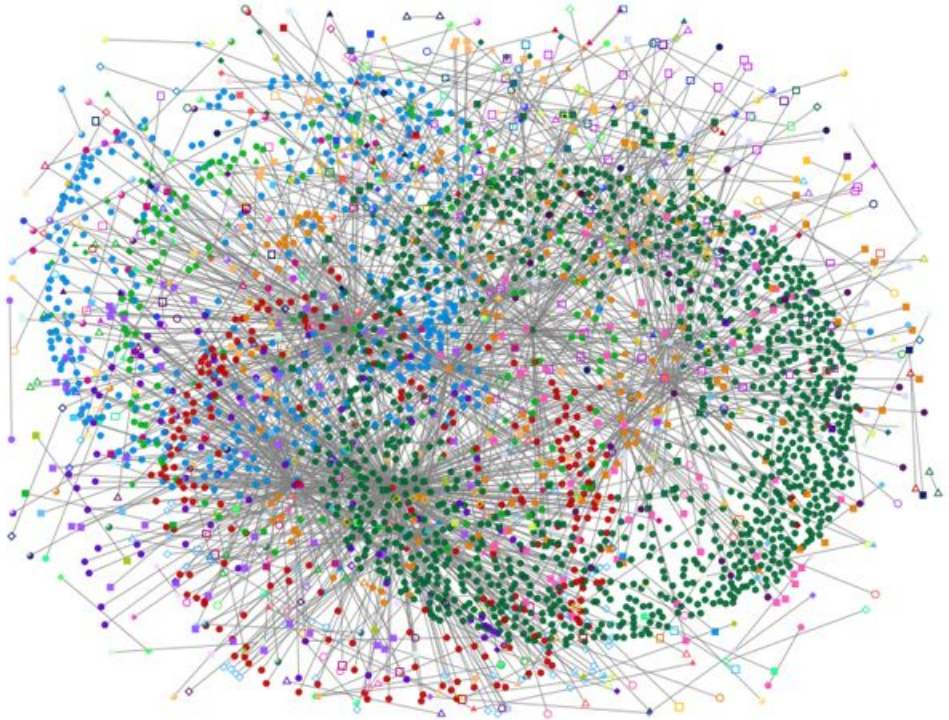
Part of Responsible & Safe AI course on NPTEL

Graphs

Molecules as graphs



Transaction Networks as graphs

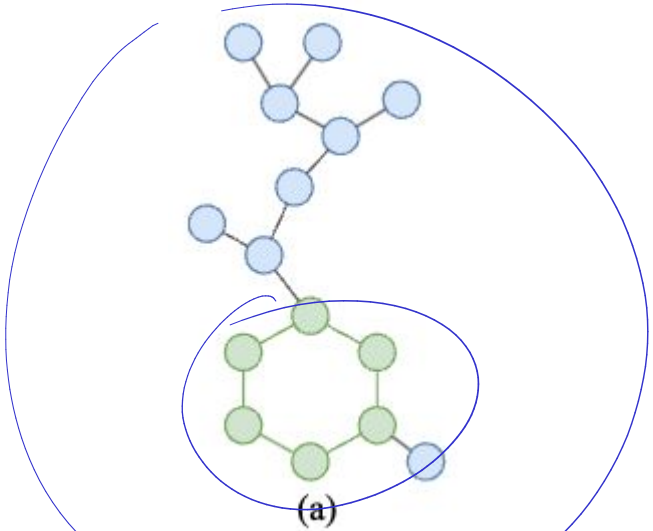


Explainability

With graphical data present in many high-risk applications, it is important that Graph Neural Network outputs are interpretable

Recent works have explored explaining GNNs and aligning them to our expectations, leading to Graph Explainers.

Important in toxicity detection of molecules, drug prediction, fraud detection, etc.



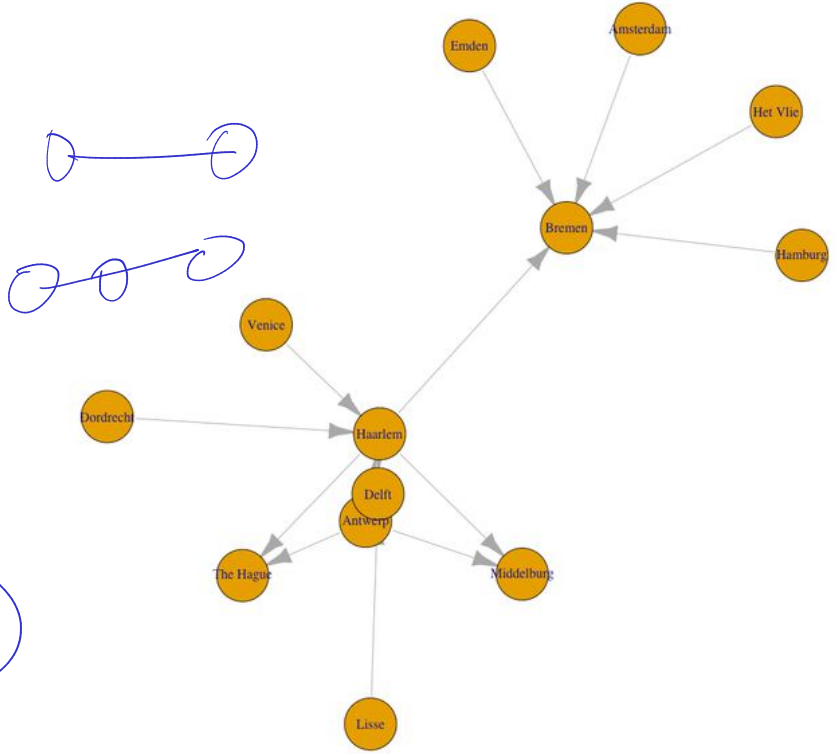
The task here is prediction of benzene in a molecule.

In this figure, we see that the “correct” explanation is the green ring here

Graph Limitations

Graphs as a data structure have an inherent limitation: they can only model pairwise relationship between nodes.

Due to this, it is hard for Graph Explainers to capture such interactions while explaining the outputs of GNNs.



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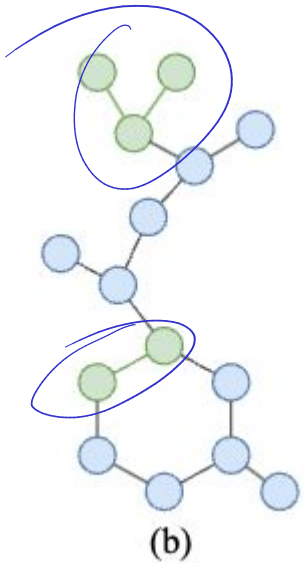
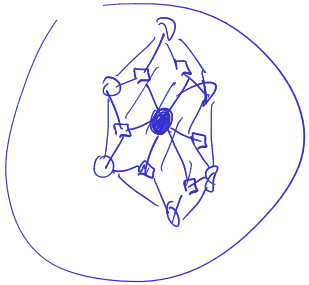


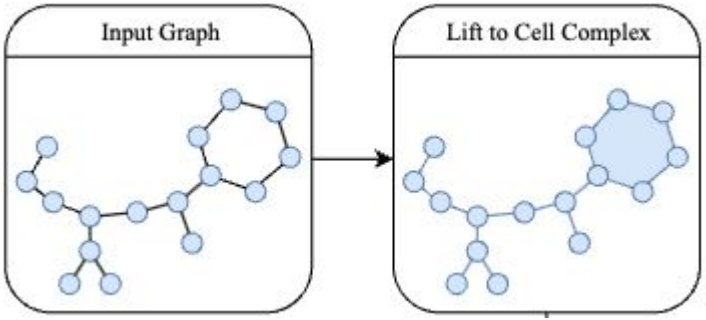
Output of GNNExplainer on the task introduced previously

Cell Complexes



To overcome this limitation, we use cell complexes

Cell complexes are a higher-order generalisation of graphs, which can capture interactions between multiple nodes.

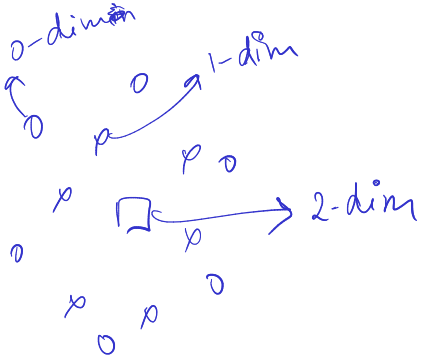


Cell Complexes

Important Definitions:

Notation	Description
G	A general graph
V	Set of all vertices in a graph
E	Set of all edges in a graph
$G(V, E)$	A graph with vertices V and edges E
X	A general cell complex
$X^{(p)}$	p-skeleton of a cell complex
c, $c^{(p)}$	general cell, cell of dimension p
$C^{(p)}$	A p-chain in a given cell complex
C	Set of all p-chains in a cell complex
σ_{c_1,c_2}	A general boundary relation
Σ	Set of all boundary relations
$X(C, \Sigma)$	A cell complex defined by C and Σ

Definition 3.1 (p-cell)**.** A p-cell $c^{(p)}$ in a cell complex refers to an element of dimension p. In analogy to traditional graphs where we have vertices (0-dimensional) and edges (1-dimensional), cell complexes include these and extend to higher dimensions.



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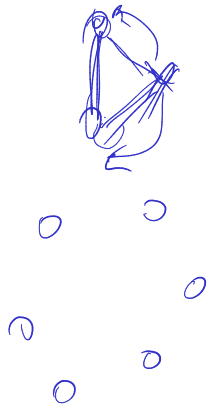
Definition 3.2 (*boundary/coboundary*)**.** In a cell complex, a p-cell $c^{(p)}$ is considered a *face* or *boundary* of a $(p+1)$-cell $c^{(p+1)}$ if the set of points composing $c^{(p)}$ is a subset of those composing $c^{(p+1)}$. Conversely, $c^{(p+1)}$ is referred to as the *coface* or *coboundary* of $c^{(p)}$.

Definition 3.3 (p-chain)**.** In a given cell complex, a p-chain $C^{(p)}$ is simply defined as the set of all p-dimensional cells. The general set union of all such $C^{(p)}$ is denoted by C.



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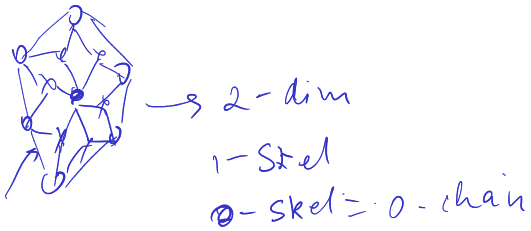
Definition 3.4 (p-skeleton)**.** The p-skeleton of a cell complex X is defined as the subcomplex $X^{(p)}$ consisting of cells of dimension at most p. Using this definition, we see that $X^{(0)}$ is the set of all vertices and $X^{(1)}$ is the set of all vertices and edges which precisely make up the underlying graph.

Definition 3.5 (*boundary relation*)**.** Within a cell complex, a boundary relation σ is analogous to an edge in traditional graphs. It connects two cells, either of the same dimension (horizontal boundary relation) or different dimensions (vertical boundary relation). A horizontal boundary relation $\sigma_{c_1^{(p)},c_2^{(p)}}$ links two p-cells that share a common *boundary* or *coboundary*, whereas vertical boundary relations $\sigma_{c_1^{(p)},c_2^{(p+1)}}$ link a p-cell to its corresponding *boundaries* or *coboundaries*. In this work, we further restrict the boundary relations to be undirected, implying $\sigma_{c_1,c_2} = \sigma_{c_2,c_1}$.



Cell Complexes

While cell complexes can model intricate relationships, this comes with additional computational costs. We see that the size of a conventional cell complex will scale *quadratically* as the size of the graph increases.

We formally show this in the next slide.

Cell Complexes

Theorem 3.1. *For a graph $G(V, E)$ with adjacency matrix A having cycles of length at most K, let W_k represent the number of closed walks of length k which are not k-cycles. Let $deg(v)$ represent the degree of a node v in the graph. The corresponding cell complex X will have cells C and boundary relations Σ such that*

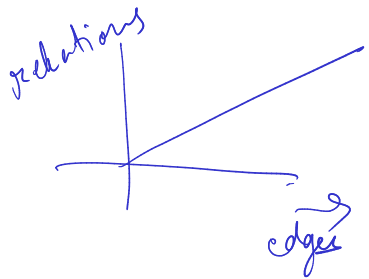
$$|C| = |V| + |E| + \sum_{k=3}^{K} \frac{1}{2k}[tr(A^{(k)}) - W_k] \quad (1)$$

$$|\Sigma| \geq 3|E| + \frac{1}{2}\sum_{k=3}^{K}[tr(A^{(k)}) - W_k] + \sum_{v \in V} \binom{deg(v)}{2} \quad (2)$$

Cell Complexes

While complexes can model intricate relationships, this comes with additional computational costs. We see that the size of a conventional cell complex will scale *quadratically* as the size of the graph increases.

However, we find that if we strategically remove specific types of boundary relations, we can bring this down to *linear* complexity.

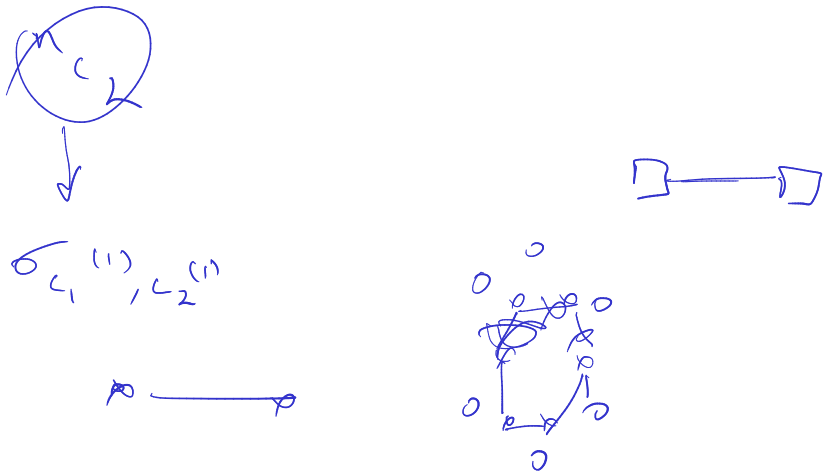


Cell Complexes

Equation (2) shows that asymptotically, the size of Σ grows *quadratically* with $|E|$, due to the last term in the equation. This term is precisely the number of boundary relations that are present between two edges in the graph, which are represented by $\sigma_{c_1^{(1)},c_2^{(1)}}$. To preserve the scalabilty and complexity of FORGE, we further restrict how we create cell complexes from graphs, and drop all boundary relations of the form $\sigma_{c_1^{(p)},c_2^{(p)}}$ where $p \geq 1$ from our construction of cell complexes. Doing this reduces Equation (2) to:

$$|\Sigma| = 3|E| + \frac{1}{2}\sum_{k=3}^{K}[tr(A^{(k)}) - W_k] \quad (3)$$

This operation ensures that $|\Sigma|$ increases *linearly* with $|E|$, making cell complexes much more scalable.



Cell Complexes

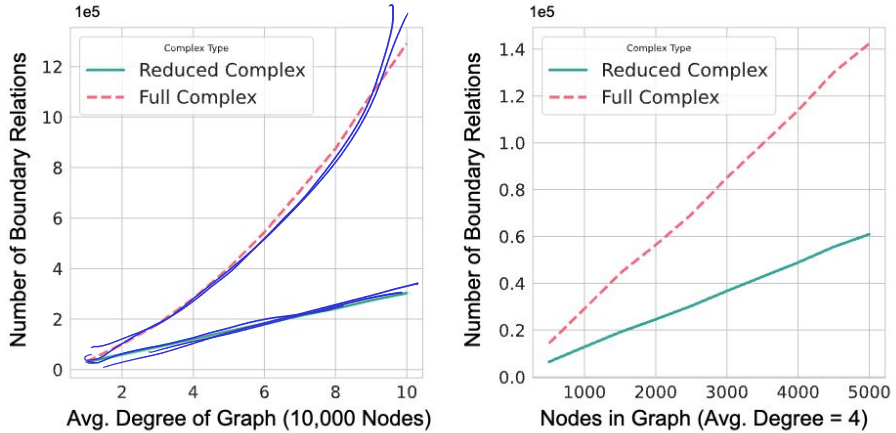
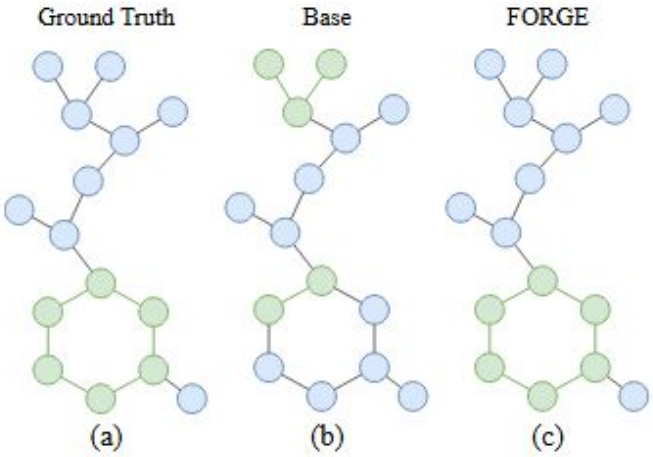


Figure 3: The variation of $|\Sigma|$ for a conventional cell complex and our proposed reduced cell complex with increasing $|E|$ (left) and increasing $|V|$ (right), showing that our proposed variation is more space efficient.

FORGE

FORGE (Framework For Higher-Order Representations In Graph Explanations) leverages complexes to improve explanations.

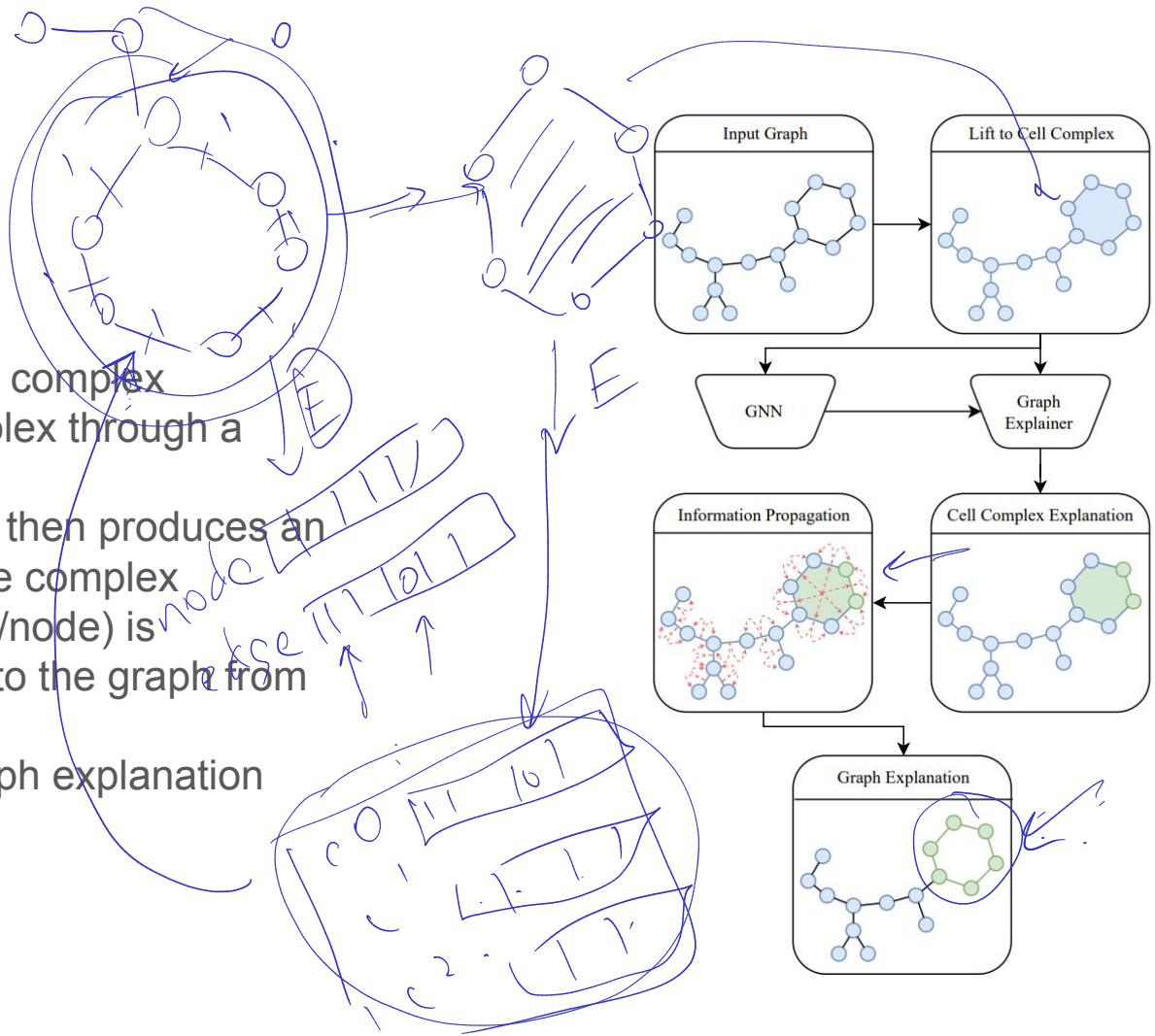
We show that integrating explainers with explicit groupwise interactions through complexes results in better and more faithful explanations over graphs.



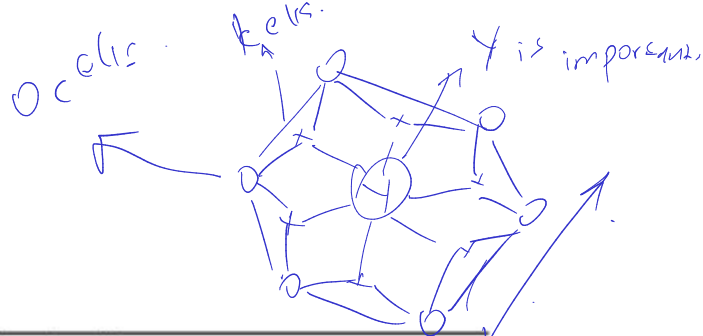
FORGE produces better explanations when groupwise interactions become important

FORGE

1. Lift graph to a cell complex
2. Run the cell complex through a GNN
3. A graph explainer then produces an explanation for the complex
4. Importance (edge/node) is propagated back to the graph from the complex
5. Resulting in a graph explanation



Lifting the Graph

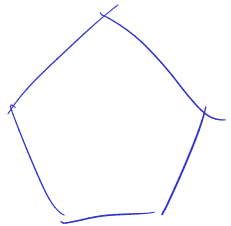


1. All nodes are 0-cells
2. Edges are 1-cells, which are represented as augmented nodes connected to the original nodes
3. Cycles are 2-cells, which are represented as augmented nodes connected to all edges that make up that cycle
4. The resulting augmented graph represents the complex

Algorithm 1: Lifting algorithm

Input: $G(V, E)$
Output: $X(C, \Sigma)$

$C^{(0)} \leftarrow \phi, C^{(1)} \leftarrow \phi, C^{(2)} \leftarrow \phi, \Sigma \leftarrow \phi$
for $e_{u,v} \in E$ **do**
  Add u, v to $C^{(0)}$
  Add $e_{u,v}$ to $C^{(1)}$
  Add $\sigma_{u,v}, \sigma_{u,e_{u,v}}, \sigma_{v,e_{u,v}}$ to Σ
end for
for $c \in$ Set of Cycles in G **do**
  Add c to $C^{(2)}$
  for $e_{u,v} \in c$ **do**
    Add $\sigma_{e_{u,v},c}$ to Σ
  end for
end for
$C \leftarrow C^{(0)} \cup C^{(1)} \cup C^{(2)}$
return $X(C, \Sigma)$



Info Prop

How do we make a graph explanation, from a complex explanation?

We propagate information back to the original graph, from the complex, in reverse-message passing direction.

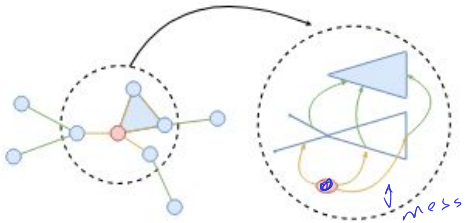


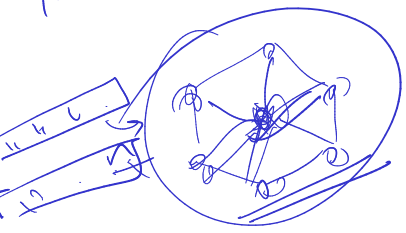
Figure 4: Example of a computation cell complex. The figure on the left shows 2-hop horizontal message passing, while the figure on the right represents 2-hop vertical message passing, introduced by FORGE.

Algorithm 2: Hierarchical Propagation

Input: $\mathcal{M}_X$
Parameters: α_c, α_e
Output: $\mathcal{M}$

for $c^{(2)} \in C^{(2)}$ **do**
  for all $\sigma_{c^{(1)},c^{(2)}}$ containing $c^{(2)}$ **do**
    $\mathcal{M}_X[c^{(1)}] \leftarrow \mathcal{M}_X[c^{(1)}] + (\mathcal{M}_X[c^{(2)}] - 0.5) \times \alpha_c$
  end for
end for
for $c^{(1)} \in C^{(1)}$ **do**
  for all $\sigma_{c^{(0)},c^{(1)}}$ containing $c^{(1)}$ **do**
    $\mathcal{M}_X[c^{(0)}] \leftarrow \mathcal{M}_X[c^{(0)}] + (\mathcal{M}_X[c^{(1)}] - 0.5) \times \alpha_e$
  end for
end for
$\mathcal{M} \leftarrow \mathcal{M}_X[C^{(0)}]$
return $\mathcal{M}$

Results

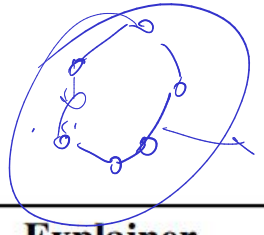


Datasets	GNNExplainer		GraphMask		GradExplainer		PGMExplainer		SubgraphX		Random
	B	F	B	F	B	F	B	F	B	F	
Benzene	0.456	**0.772**	0.276	0.378	0.167	0.353	0.109	0.198	0.450	0.614	0.194
AlkCarb	0.054	0.130	0.048	0.055	0.114	0.217	0.095	**0.304**	0.002	0.011	0.050
FluoCarb	0.207	**0.441**	0.077	0.230	0.233	0.439	0.115	0.300	0.079	0.095	0.154
Mutag	**0.380**	0.339	0.127	0.163	0.172	0.218	0.114	0.233	0.079	0.095	0.112
Bull/Square	0.126	0.433	0.082	0.241	0.179	0.298	0.080	0.150	0.355	**0.447**	0.145
House/Hex	0.107	0.478	0.115	0.271	0.199	0.410	0.088	0.158	0.346	**0.617**	0.165
Wheel/House	0.102	0.361	0.233	0.378	0.169	0.426	0.083	0.195	0.246	**0.549**	0.194
Cube/Wheel	0.114	0.339	0.183	0.402	0.119	**0.494**	0.091	0.178	0.397	0.489	0.221

Table 2: Graph Explanation Accuracy (GEA) (↑) scores for baseline explainers **(B)** against their FORGE variants **(F)** across all datasets, with FORGE improving performance across various baselines. Best result for each dataset is highlighted in **bold**. Underlined values represent the better result between a base explainer and its FORGE variant.

Results

We also show that FORGE produces explanation more faithful to the underlying GNN



Explainer	GEF(↓) B	GEF(↓) F
GNNExplainer	$0.189_{\pm 0.04}$	$\mathbf{0.083_{\pm 0.02}}$
GraphMask	$0.051_{\pm 0.03}$	$\mathbf{0.028_{\pm 0.02}}$
GradExplainer	$0.389_{\pm 0.13}$	$\mathbf{0.078_{\pm 0.05}}$
PGMExplainer	$\mathbf{0.204_{\pm 0.05}}$	$0.234_{\pm 0.03}$
SubgraphX	$0.008_{\pm 0.01}$	$\mathbf{0.007_{\pm 0.00}}$
Random	$0.124_{\pm 0.04}$	-

Table 3: Graph Explanation Faithfulness (GEF) Scores for the AlkaneCarbonyl Dataset. FORGE enhanced explainers generate explanations that are comparable or more faithful to the underlying GNN. Values in **bold** indicate best performance.

Observations / Discussion

Perturbation-based methods benefit the most from our framework, with FORGE applied to GNNExplainer generally delivering the best performance on real-world datasets, while FORGE on SubgraphX excels in synthetic datasets.

Some Explainers in their default form perform worse than the Random baseline. However, after applying FORGE, all explainers consistently surpass the Random baseline, achieving significantly improved performance

Our results reveal substantial variability in explainer effectiveness depending on the graph types and tasks. No single method consistently outperforms others across all datasets, suggesting the importance of choosing explainers tailored to specific problem domains.

Ablations

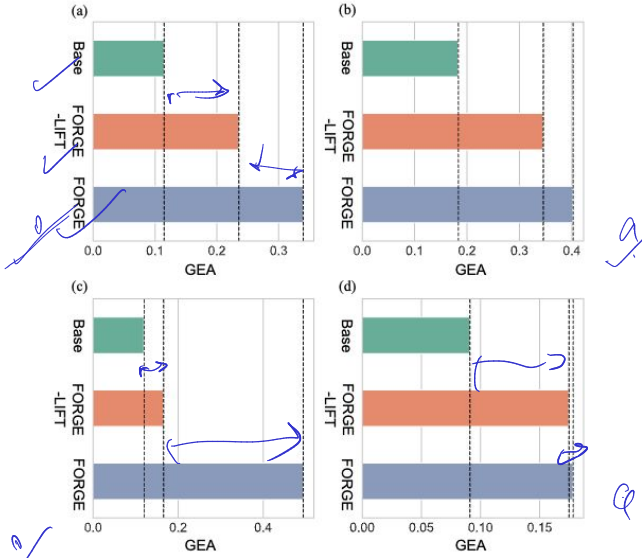


Figure 6: Results of ablations on FORGE Components for **(a)** GNNExplainer, **(b)** GraphMaskExplainer, **(c)** GradExplainer, **(d)** PGMExplainer on Synth-Wheel/Cube dataset. Both Lifting and Information Propagation contribute significantly to increase in explanation accuracy.

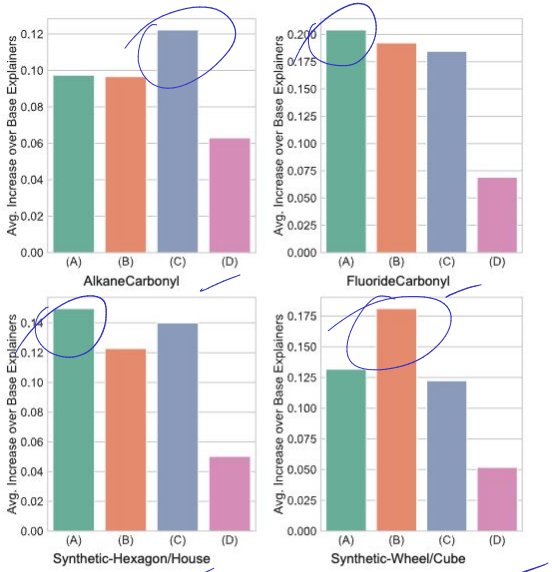


Figure 7: Ablation results for different propagation methods on various datasets, for all baseline explainers. The y-axis represents the average absolute increase in GEA over base explainers. **(A)** Hierarchical Prop, **(B)** Direct Prop, **(C)** Activation Prop, and **(D)** Entropy Prop.

Takeaways

- Cell Complexes are powerful tools to model groupwise interactions in graphs
- FORGE exploits cell complexes resulting in human interpretable and improved explanations over graphs
- Explainers are often task dependent and so ensure you test multiple explainers before choosing

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